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13. ABSTRACT (Maximum 200 words) <p>This research involves theoretical studies of the chemical and fluid-mechanical phenomena which make turbulent combustion in high-speed flows different from such combustion in low-speed flows. Finite-rate chemistry plays a significant role in high-speed flows because of the small ratios of flow times to chemical times. The studies address ignition and extinction phenomena in nonpremixed turbulent combustion of hydrogen-air systems by both numerical and asymptotic methods. Attention also is paid to effects of compressibility in high-speed turbulent combustion, with consideration given to interdispersal configurations of shocklets and flamelets. Efforts are made to provide a firmer foundation for the modeling of high-speed turbulent reacting flows, to aid in the development of a formulation which gives results that can be compared with experiments on turbulent combustion.</p>				
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INTRODUCTION

Uncertainties about turbulent combustion in hydrogen-air systems have an impact on our abilities to achieve successful designs of supersonic combustion devices for the National Aerospace Plane, for example. Prior to initiation of the present research, it was not known whether the combustion was more likely to occur in reaction-sheet or distributed-reaction regimes, and common practice was to assume the latter and employ laminar chemical kinetics in routines based on computational fluid mechanics. As will be seen below, estimates suggest that this is a poor procedure since the reaction-sheet regime is more prevalent than the distributed-reaction regime. The present research was initiated because it was felt desirable to try to determine the regimes more firmly and to develop improved methods for accounting for the chemical kinetics of the combustion.

RESEARCH OBJECTIVES

The objective of this research is to improve understanding of the chemical kinetics and fluid dynamics of turbulent combustion in high-speed flows. Supersonic combustion in hydrogen-air mixtures is being addressed by theoretical approaches that distinguish between reaction-sheet and distributed-reaction regimes. The work seeks to identify effects of compressibility in turbulent combustion, methods for including compressibility in theoretical analyses, and reduced chemical-kinetic mechanisms appropriate for supersonic combustion. The results may help to enhance capabilities of reasonable computations of high-speed turbulent reacting flows.

ACCOMPLISHMENTS

Regimes of Turbulent Combustion

The work on the present project has been addressing flamelet regimes rather than distributed-reaction regimes of turbulent combustion. The motivation for focusing on flamelets stems from the initial evaluation, under the previous grant, indicating that in the application to aerospace propulsion, the hydrogen-air system lies in the reaction-sheet regime. Those initial estimates were made prior to development of the extensive data base on hydrogen-air diffusion flames, from the previous grant. Because of this, it seemed reasonable at the outset to reevaluate the combustion regimes, on the basis of the new information that has now been accumulated. The results of this reevaluation reaffirm that reaction-sheet flamelet regimes are most relevant. In comparison with the original estimates, there has been a narrowing of the most probable range and a displacement towards the distributed-reaction regime as a consequence of improved chemical-kinetic and combustion information. Therefore, attention continues to be placed on flamelets.

Ignition in Hydrogen-Air Mixtures

Previous work addressed steady burning and extinction in hydrogen-air systems but did not consider the ignition branch of the diffusion-flame S curve. Autoignition of hydrogen with hot air is of fundamental interest in high-speed propulsion; for instance, in a supersonic combustor the fuel jet is expected to be injected into and ignited by a stream of hot air heated by shocks. Typical studies of ignition focus on the chemistry with little or no attention being paid to the fluid dynamics. Complex interactions which are likely

to play an important role in the ignition processes in real flow are thus ignored. To help to understand these interactions, current attention is focused on the ignition of a cold jet of hydrogen impinging against an opposed jet of heated air.

The problem is reduced to a two-point boundary-value problem for ordinary differential equations. The numerical solution to the discretized equations, normally obtained employing Newton's method or a variant thereof, encounters difficulties in the neighborhood of turning points where the derivative of the solution with respect to a parameter of the problem becomes infinite (for example, at the extinction condition). To circumvent these difficulties, a modification of the basic algorithm is introduced in the present work, employing a path-tracing continuation method of Smooke, in which points on the arc of solutions are computed. This method has now succeeded in generating the ignition branch.

Computations began with the 21-step mechanism which was used for extinction studies reported earlier. Numerical integrations were also performed with a different chemical scheme proposed by Smooke and his coworkers. For dilute hydrogen flames at one atmosphere pressure, a large discrepancy in the extinction and ignition strain rates was observed with increasing feed temperature of the air stream. Furthermore, thermal diffusion was seen to play a surprisingly important role in diluted flames. In view of these unexpected preliminary results, a critical assessment of the reaction rates was deemed warranted. After an extensive survey of the literature and discussions with other researchers, especially Yetter, the 21-step chemical-kinetic scheme with associated rate parameters shown in Table 1 was selected as representing the best information currently available.

To test the updated chemistry, flame speeds for hydrogen-air, wet CO and methane-air mixtures were calculated. The agreement between theory and experiment is excellent over a wide range of initial conditions for the hydrogen-air flame. A flame speed of 38.6 cm/s for stoichiometric methane-air flames was obtained, in good agreement with the experimental value of 38-40 cm/s. Of particular interest in the new chemical scheme is the rate of the chain-branching reaction $H + O_2 \rightarrow OH + O$, which is based on the recent Stanford shock-tube experiments. The new rate provides a slightly larger radical pool, and unlike the rate recommended by Baulch et al. in their recent 1992 review, exhibits the correct direction of the temperature dependence for the reverse reaction $OH + O \rightarrow H + O_2$ in the temperature range of 500-3000 K.

Calculations to characterize the ignition of hydrogen-air mixtures over a wide range of conditions of interest in high-speed propulsion devices are now being performed with the updated chemical scheme.

Structures of Counterflow Diffusion Flames with Small Stoichiometric Mixture Fractions

Asymptotic methods were used to evaluate a characteristic diffusion time for counterflow diffusion flames, a quantity of utmost importance in analyses of flame structure and extinction. Attention was restricted to the important limit of small values of the stoichiometric mixture fraction, which resulted in large values of the stream function at the reaction sheet, a quantity which was then employed as a large expansion parameter. Three distinct layers were identified inside the viscous layer: (1) a convective-diffusive

layer on the oxidizer side of the reaction sheet, (2) a rotational inviscid layer on the fuel side of the reaction sheet, and (3) a fuel-product mixing layer in the vicinity of the stagnation plane; all three of these layers were analyzed and matched. The matching produced analytic expressions for the stream function and mixture fraction at the reaction sheet and corrected formulas for the characteristic diffusion time previously derived on the basis of constant-density or nonreactive-mixing assumptions. Comparison between analytical and numerical results demonstrate that the analytical results obtained from the present analysis provide accurate expressions for the characteristic diffusion times and stoichiometric scalar dissipation rates. The results provide improved predictions of the diffusion-flame structure and extinction.

Nonpremixed Flames in Stagnating Turbulence

It is becoming widely recognized that the study of flames in stagnating turbulence provides a powerful vehicle for examining fundamental issues in turbulent combustion. For the present discussion the flow of interest consists of two coaxial, axisymmetric and closely spaced jets within which a turbulence-generating grid is installed. By changing the mean velocity from each jet, the entire range of chemical behavior from equilibrium to extinction can be covered in one experimental setup. The initial experimental investigations of these flames were confined to premixed systems, i.e. to a turbulent reactant stream either impinging on a wall or opposing another reactant stream, but recently preliminary results of an experiment involving a flame in a turbulent methane stream opposing a turbulent airstream have been reported. Since the only theory of flames in stagnating turbulence is concerned with premixed systems, an analysis of the nonpremixed case has been started under the present program.

The initial results are based on the thin-flame approximation and on chemical equilibrium, with matching to outer zones imposed on each side of the flame. This approximation involves two nonreactive streams impinging on the opposite sides of a turbulent flame whose thickness is small compared with the jet spacing. The resultant calculated temperature distribution exhibits a peak value and general shape in excellent agreement with experiments, but the predicted thickness in physical space is an order of magnitude too small. In brief, the thin-flame approximation is not applicable to the experimental conditions. The combination of heat release and of turbulent length scale preclude quantitative comparison of theory with these experiments. Accordingly, an alternative analysis has been developed, describing in one set of equation the entire flow from one jet exit plane to the other. The numerical treatment of this new set of equation is underway. Initial application will be to the methane-air system, to permit comparison with available experimental data; if the agreement is satisfactory, with or without refinements to the theory, the analysis will then be applied to the hydrogen-air system. Additional studies along these lines involve the effects of finite chemical rates, so that extinction and ignition can be analyzed. These studies will clearly relate to the flamelet analyses described earlier.

PUBLICATIONS

1. G. Balakrishnan, C. Treviño, and F. Mauss. Asymptotic structure of hydrogen-air diffusion flames. *Combustion and Flame*, 91 (3-4):246-256, December 1992.

2. E. Gutheil, G. Balakrishnan, and F. A. Williams. Structure and extinction of hydrogen-air diffusion flames. In N. Peters and B. Rogg, editors, *Reduced Kinetic Mechanisms for Application in Combustion Systems*. Springer Verlag, Berlin, 1993.
3. G. Balakrishnan. *Studies of Hydrogen-Air Diffusion Flames and of Compressibility Effects, Related to High Speed Propulsion*. PhD thesis, University of California San Diego, September 1992.
4. J. S. Kim and F. A. Williams. Structures of flow and mixture fraction fields for counterflow diffusion flames with small stoichiometric mixture fractions. *SIAM Journal on Applied Mathematics*, 53(6), December 1993.

PERSONNEL

Percentage Time

Professor P. A. Libby	Principal Investigator	15%
Professor F. A. Williams	Principal Investigator	15%
Mr. G. Balakrishnan	PhD Student to October, 1992	50%
	Postgraduate Researcher after October, 1992	100%

INTERACTIONS

Related talks given by the PIs at meetings and at visits during the reporting period are:

"Deflagration of Nitramines", BRL, Aberdeen, April 8, 1992.

"Turbulent Combustion", 12th Kovasznay Distinguished Lecturer, University of Houston, April 16, 1992.

"NO_x Production in Large Turbulent Diffusion Flames," University of California, Berkeley, May 4, 1992.

"The Role of Theory in Combustion Science," Hottel Plenary Lecture, Twenty-Fourth International Symposium on Combustion, The University of Sydney, July 5, 1992.

"Theory of Nitramine Deflagration", Materials Research Laboratory, DSO, Adelaide, July 14, 1992.

"The Role of Turbulence Modeling in Combustion", Stanford University, July 23, 1992.

"Advances in Modeling of Turbulent Combustion", Sixth Toyota Conference, Mikkabi, October 11, 1992.

"Hydrogen Diffusion-Flame Studies for High-Speed Propulsion", ICASE, NASA, Langley, October 22, 1992.

"High Speed Turbulent Combustion", ICASE workshop, NASA, Langley, October 11-13, 1992.

Chair of a Session at First International Symposium on Liquid Rocket Combustion Instability, Penn State, January 18, 1993.

"Supercritical Combustion of Multicomponent Droplets," Phillips Laboratory, Edwards Air Force Base, March 5, 1993.

"Flames in Stagnating Turbulence", STAR Workshop, University of California, Davis, March 18 and 19, 1993

Various discussion with Jesse Crump, Jay Levine and Doug Talley of Phillips Laboratory on combustion and instability problems.

INVENTIONS

none

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Table 1: Specific Reaction-Rate Constants for the Hydrogen-Oxygen Reaction System Adopted in the Present Study.

No.	Reactions	A ¹	n ¹	E ¹
1	$\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O}$	3.52×10^{16}	-0.7	17070
2	$\text{H}_2 + \text{O} \rightleftharpoons \text{OH} + \text{H}$	5.06×10^4	2.67	6290
3	$\text{OH} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$	$k = 5.46 \times 10^{11} \exp(0.00149T)$		
4	$\text{H}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}$	1.17×10^9	1.3	3626
5 ²	$\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$	6.76×10^{19}	-1.42	0
6	$\text{H} + \text{HO}_2 \rightarrow \text{OH} + \text{OH}$	1.70×10^{14}	0.0	874
7	$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	4.28×10^{13}	0.0	1411
8	$\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$	2.89×10^{13}	0.0	497
9 ³	$\text{H} + \text{H} + \text{M} \rightarrow \text{H}_2 + \text{M}$	1.80×10^{18}	-1.0	0
10 ²	$\text{H} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M}$	2.20×10^{22}	-2.0	0
11	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	3.02×10^{12}	0.0	1390
12 ⁴	$\text{H}_2\text{O}_2 + \text{M} \rightleftharpoons \text{OH} + \text{OH} + \text{M}$	1.20×10^{17}	0.0	45500
13	$\text{H}_2\text{O}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{HO}_2$	7.08×10^{12}	0.0	1430
14	$\text{O} + \text{HO}_2 \rightleftharpoons \text{OH} + \text{O}_2$	2.00×10^{13}	0.0	0
15	$\text{H} + \text{HO}_2 \rightleftharpoons \text{O} + \text{H}_2\text{O}$	3.10×10^{13}	0.0	1720
16 ²	$\text{H} + \text{O} + \text{M} \rightleftharpoons \text{OH} + \text{M}$	6.20×10^{16}	-0.6	0
17 ²	$\text{O} + \text{O} + \text{M} \rightleftharpoons \text{O}_2 + \text{M}$	6.17×10^{15}	-0.5	0
18	$\text{H}_2\text{O}_2 + \text{H} \rightleftharpoons \text{H}_2\text{O} + \text{OH}$	1.00×10^{13}	0.0	3590
19	$\text{H}_2\text{O}_2 + \text{H} \rightleftharpoons \text{HO}_2 + \text{H}_2$	4.79×10^{13}	0.0	7950
20	$\text{O} + \text{OH} + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$	1.00×10^{16}	0.0	0
21	$\text{H}_2 + \text{O}_2 \rightleftharpoons \text{OH} + \text{OH}$	1.70×10^{13}	0.0	47780

^a Units: mol/cm³, s⁻¹, K, cal/mol; rates for reverse steps obtained from JANAF thermochemical equilibrium data.

^b Chaperon Efficiencies: H₂: 2.5, H₂O: 12.0, O₂: 1.0 and N₂: 1.0

^c Chaperon Efficiencies: H₂: 1, H₂O: 6.5, O₂: 0.4 and N₂: 0.4

^d Chaperon Efficiencies: H₂: 2.5, H₂O: 15.0, O₂: 1.0 and N₂: 1.0